Gilles A De Wijs

List of Publications by Year
in descending order

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111 papers	5,226 citations	81743 39 h-index	88477 70 g-index
117 all docs	117 docs citations	117 times ranked	6704 citing authors

#	Article	IF	Citations
1	thermodynamic metastability, and optical properties of anion-disordered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^’</mml:mo><mml:mn>2</mml:mn><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>		

#	Article	IF	Citations
19	Li intercalation in graphite: A van der Waals density-functional study. Physical Review B, 2014, 90, .	1.1	63
20	Quantum confinement and band offsets in amorphous silicon quantum wells. Physical Review B, 2014, 90, .	1.1	6
21	Carbon Support Effects on the Hydrogen Storage Properties of LiBH₄ Nanoparticles: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 5102-5109.	1.5	12
22	Anionogenic Mixed Valency in KxBa1â€“xO2â^Ï´. Inorganic Chemistry, 2014, 53, 496-502.	1.9	4
23	Phonons and electronâ€phonon coupling in grapheneâ€hâ€BN heterostructures. Annalen Der Physik, 2014, 526, 381-386.	0.9	40
24	Interactions of adsorbed CO2 on water ice at low temperatures. Physical Chemistry Chemical Physics, 2014, 16, 15630.	1.3	25
25	Stripline ⁷⁵As NMR Study of Epitaxial IIIâ€“V Semiconductor Al_{0.5}Ga_{0.5}As. Journal of Physical Chemistry C, 2014, 118, 13394-13405.	1.5	4
26	The electronic structure of organicâ€“inorganic hybrid compounds: (NH₄)₂CuCl₄, (CH₃NH₃)₂CuCl₄and (C₂H₅NH₃)₂CuCl₄. Journal of Physics Condensed Matter, 2013, 25, 295502.	0.7	39
27	Role of Magnetism in Catalysis: RuO₂ (110) Surface. Journal of Physical Chemistry C, 2013, 117, 6353-6357.	1.5	98
28	First-Principles Study of Structural Prototypes for NaAlH4: Elevated Pressure Polymorph in Symmetry Fmm2 Leads to a Single-Step Decomposition Pathway. Journal of Physical Chemistry C, 2013, 117, 8864-8870.	1.5	3
29	Excess manganese as the origin of the low-temperature anomaly in NiMnSb. Physical Review B, 2013, 88, .	1.1	9
30	Finite-field implementation of NMR chemical shieldings for molecules: Direct and converse gauge-including projector-augmented-wave methods. Journal of Chemical Physics, 2013, 139, 014109.	1.2	13
31	R<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>Â·</mml:mo></mml:math>p subband structure of the LaAlO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>interface. Physical Review B, 2013, 88, .	1.1	25
32	Switchable Fermi surface sheets in greigite. Physical Review B, 2012, 86, .	1.1	12
33	First-Principles Study of LiBH4Nanoclusters and Their Hydrogen Storage Properties. Journal of Physical Chemistry C, 2012, 116, 18038-18047.	1.5	23
34	Intrinsic defects and dopants in LiNH2: a first-principles study. Physical Chemistry Chemical Physics, 2011, 13, 6043.	1.3	15
35	Native Defects and the Dehydrogenation of NaBH4. Journal of Physical Chemistry C, 2011, 115, 24429-24434.	1.5	13
36	Hydrogen bonding and chemical shift assignments in carbazole functionalized isocyanides from solid-state NMR and first-principles calculations. Physical Chemistry Chemical Physics, 2011, 13, 13082.	1.3	28

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37	Mixed Magnetism for Refrigeration and Energy Conversion. Advanced Energy Materials, 2011, 1, 1215-1219.	10.2	227
38	Optical response of the sodium alanate system:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="italic">GW</mml:mi><mml:mrow><mml:mn>0</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>-BSE calculations and thin film measurements. Physical Review B, 2011, 83, .	1.1	20
39	Atomistic models of hydrogenated amorphous silicon nitride from first principles. Physical Review B, 2010, 82, .	1.1	22
40	Structural models of aâ€Si:H with a low defect concentration: A firstâ€principles molecular dynamics study. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 605-608.	0.8	2
41	First-principles modelling of magnesium titanium hydrides. Journal of Physics Condensed Matter, 2010, 22, 074208.	0.7	12
42	Tuning the Hydrogen Storage in Magnesium Alloys. Journal of Physical Chemistry Letters, 2010, 1, 1982-1986.	2.1	25
43	A solid-state NMR and DFT study of compositional modulations in AlxGa1âˆ’xAs. Physical Chemistry Chemical Physics, 2010, 12, 11517.	1.3	29
44	Publisher's Note: Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors [Phys. Rev. B79, 085203 (2009)]. Physical Review B, 2009, 79, .	1.1	8
45	First-principles study of the optical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2009, 79, .	1.1	20
46	Amorphous Semiconductors Studied by First-principles Simulations: Structure and Electronic Properties. Materials Research Society Symposia Proceedings, 2009, 1153, 1.	0.1	1
47	First-principles study of hydrogenated amorphous silicon. Physical Review B, 2009, 79, .	1.1	61
48	Hydrogen Storage by Polylithiated Molecules and Nanostructures. Journal of Physical Chemistry C, 2009, 113, 8997-9002.	1.5	39
49	DFT Study of Planar Boron Sheets: A New Template for Hydrogen Storage. Journal of Physical Chemistry C, 2009, 113, 18962-18967.	1.5	130
50	Tunable hydrogen storage in magnesiumâ€“transition metal compounds: First-principles calculations. Physical Review B, 2009, 79, .	1.1	48
51	Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors. Physical Review B, 2009, 79, .	1.1	105
52	Electronic Band Structure of Tetraceneâˆ’TCNQ and Peryleneâˆ’TCNQ Compounds. Journal of Physical Chemistry A, 2008, 112, 2497-2502.	1.1	46
53	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Be</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow> Physical Review B, 2008, 77, .	1.1	31
54	A Density Functional Study of Î±-Mg(BH4)2. Chemistry of Materials, 2008, 20, 4952-4956.	3.2	76

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55	Theoretical Study of the Stable Radicals Galvinoxyl, Azagalvinoxyl and Wursterâ€™s Blue Perchlorate in the Solid State. Journal of Physical Chemistry A, 2008, 112, 7734-7738.	1.1	15
56	Spin Tunneling in Junctions with Disordered Ferromagnets. Physical Review Letters, 2008, 100, 057205.	2.9	31
57	Work function anisotropy and surface stability of half-metallicCrO2. Physical Review B, 2008, 77, .	1.1	18
58	Ab initiostudy of the effects of transition metal doping of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Ni</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	1.1	61
59	Crystal Growth, Structure, and Electronic Band Structure of Tetraceneâ^'TCNQ. Journal of Physical Chemistry C, 2007, 111, 3486-3489.	1.5	38
60	Lattice and local-mode vibrations in anhydrous and protonized LiMn2O4 spinels from first-principles theory. Journal of Materials Chemistry, 2007, 17, 4908.	6.7	15
61	Model for the Formation Energies of Alanates and Boranates. Journal of Physical Chemistry C, 2007, 111, 9592-9594.	1.5	9
62	Thermodynamic Stability of Boron:Â The Role of Defects and Zero Point Motion. Journal of the American Chemical Society, 2007, 129, 2458-2465.	6.6	169
63	Spintronic materials based on main-group elements. Journal of Physics Condensed Matter, 2007, 19, 165203.	0.7	26
64	Optimizing performance of half-metals at finite temperature. Journal of Physics Condensed Matter, 2007, 19, 315212.	0.7	20
65	Electronic structure and optical properties of lightweight metal hydrides. Physical Review B, 2007, 75, .	1.1	120
66	The continuing drama of the half-metal/semiconductor interface. Journal Physics D: Applied Physics, 2006, 39, 793-796.	1.3	45
67	Ab Initio and Work Function and Surface Energy Anisotropy of LaB6. Journal of Physical Chemistry B, 2006, 110, 18459-18465.	1.2	74
68	Local Structure and Chemical Bonding of Protonated LixMn2O4Spinels from First Principles. Chemistry of Materials, 2006, 18, 1169-1173.	3.2	20
69	Generalised coexistence of a low work function and a stable surface: CaAl4 and BaAuIn3. Surface Science, 2006, 600, 2495-2500.	0.8	7
70	The role of the hydrogen bonding network for the shear modulus of PIPD. Polymer, 2005, 46, 9144-9154.	1.8	18
71	Quantum mechanics calculations on the diastereomeric salts of cyclic phosphoric acids with ephedrine. Computational and Theoretical Chemistry, 2005, 717, 205-214.	1.5	0
72	Geometry of {001} Surfaces of Spinel (MgAl2O4): First-Principles Simulations and Experimental Measurements. Journal of the American Ceramic Society, 2005, 88, 1544-1548.	1.9	34

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73	Tunable spin transport in CrAs: Role of correlation effects. Physical Review B, 2005, 71, .	1.1	40
74	Ab initiostudy ofMg(AlH4)2. Physical Review B, 2005, 72, .	1.1	49
75	Interrelation of Work Function and Surface Stability: The Case of BaAl4. Chemistry of Materials, 2005, 17, 3879-3882.	3.2	9
76	Anionogenic Ferromagnets. Journal of the American Chemical Society, 2005, 127, 16325-16328.	6.6	62
77	Lattice vibrations and thermal properties of carbon nitride with defect ZnS structure from first-principles calculations. Journal of Physics Condensed Matter, 2004, 16, 3027-3034.	0.7	7
78	Low work function of the (1000) Ca2N surface. Journal of Applied Physics, 2004, 96, 1751-1753.	1.1	21
79	Defects in half-metals and finite temperature. Journal of Physics Condensed Matter, 2004, 16, S5517-S5524.	0.7	37
80	Local structure and electronic properties of BaTaO2N with perovskite-type structure. Journal of Physics and Chemistry of Solids, 2003, 64, 281-286.	1.9	67
81	Weakening of a Polyethylene Chain by Methyl Side Groups. Soft Materials, 2003, 1, 223-233.	0.8	3
82	Anisotropy of the mobility of pentacene from frustration. Synthetic Metals, 2003, 139, 109-114.	2.1	125
83	Phonon spectrum and thermal properties of cubic Si3N4 from first-principles calculations. Journal of Applied Physics, 2003, 93, 5175-5180.	1.1	50
84	Modeling the Polymorphism of Pentacene. Journal of the American Chemical Society, 2003, 125, 6323-6330.	6.6	214
85	First-principles calculation of the phonon spectrum ofMgAl2O4spinel. Physical Review B, 2002, 65, .	1.1	66
86	Phonon spectrum ofZnAl2O4spinel from inelastic neutron scattering and first-principles calculations. Physical Review B, 2002, 66, .	1.1	60
87	Spin-polarization in half-metals (invited). Journal of Applied Physics, 2002, 91, 8340.	1.1	201
88	The electronic structure of tantalum (oxy)nitrides TaON and Ta3N5. Journal of Materials Chemistry, 2001, 11, 1248-1252.	6.7	178
89	Amorphous WO3: a first-principles approach. Electrochimica Acta, 2001, 46, 1989-1993.	2.6	52
90	Patterning of Si(001) with halogens: Surface structure as a function of the halogen chemical potential. Physical Review B, 2001, 64, .	1.1	23

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91	Towards 100% spin-polarized charge-injection: The half-metallic NiMnSb/CdS interface. Physical Review B, 2001, 64, .	1.1	184
92	Lithium trapping by excess oxygen inWO3:A first-principles study. Physical Review B, 2000, 62, 1508-1511.	1.1	6
93	Bond Scission in a Perfect Polyethylene Chain and the Consequences for the Ultimate Strength. Macromolecules, 2000, 33, 9098-9108.	2.2	32
94	O/N Ordering in Y2Si3O3N4 with the Melilite-type Structure from First-Principles Calculations. Chemistry of Materials, 2000, 12, 1071-1075.	3.2	27
95	Bulk and Surface Electronic Structure of the Layered Sub-Nitrides Ca2N and Sr2N. Chemistry of Materials, 2000, 12, 1847-1852.	3.2	28
96	Structure and electronic properties of amorphousWO3. Physical Review B, 1999, 60, 16463-16474.	1.1	88
97	Transport coefficients of liquids from first principles. Journal of Non-Crystalline Solids, 1999, 250-252, 82-90.	1.5	11
98	The viscosity of liquid iron at the physical conditions of the Earth's core. Nature, 1998, 392, 805-807.	13.7	259
99	First-order phase transitions by first-principles free-energy calculations: The melting of Al. Physical Review B, 1998, 57, 8223-8234.	1.1	124
100	First-principles study of chlorine adsorption and reactions onSi(100). Physical Review B, 1998, 57, 10021-10029.	1.1	50
101	Reversed spin polarization at the Co(001)-HfO2(001) interface. Physical Review B, 1998, 58, 15422-15425.	1.1	15
102	Mechanism for SiCl2Formation and Desorption and the Growth of Pits in the Etching of Si(100) with Chlorine. Physical Review Letters, 1997, 78, 4877-4880.	2.9	54
103	First principles calculations on crystalline and liquid iron at Earth's core conditions. Faraday Discussions, 1997, 106, 205-218.	1.6	106
104	Chlorine onSi(001)â˜(2Ã—1): Bridge versus Terminal Bonding. Physical Review Letters, 1996, 77, 881-884.	2.9	22
105	Electron-Ion Correlation in Liquid Metals from First Principles: Liquid Mg and Liquid Bi. Physical Review Letters, 1995, 75, 4480-4483.	2.9	36
106	Firstâ€principles molecularâ€dynamics simulation of liquid CsPb. Journal of Chemical Physics, 1995, 103, 5031-5040.	1.2	38
107	Clusters in liquid K-Tl and Cs-Tl alloys. Journal of Physics Condensed Matter, 1994, 6, A255-A260.	0.7	12
108	Ab initio molecular dynamics study of liquid Li12Si7. Journal of Non-Crystalline Solids, 1993, 156-158, 961-964.	1.5	1

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109	Structure of liquid caesium-lead alloys. Journal of Non-Crystalline Solids, 1993, 156-158, 34-37.	1.5	8
110	Nanometre superstructure in liquid alkali-thallium alloys. Journal of Physics Condensed Matter, 1993, 5, 9253-9260.	0.7	14
111	First-principles molecular-dynamics simulation of liquidLi12Si7. Physical Review B, 1993, 48, 13459-13468.	1.1	21